Characteristics of Surface Acoustic Waves in (100) AlN/64ºYX-$LiNbO_3$ Structures

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Abstract

A-axis-oriented AlN films are deposited on the 64ºYX-$LiNbO_3$ substrate by the RF magnetron sputtering method. The crystalline structure of the AlN films is determined and confirmed by X-ray diffraction. Phase velocity, coupling coefficient, and temperature coefficient of frequency (TCF) of surface acoustic waves (SAWs) in the (100) AlN/64ºYX-$LiNbO_3$ structures with different thicknesses of AlN films are measured. Simulation results show good agreement with measurement data. The research results illustrate that the increase of the thickness of AlN films will increase the SAW velocity, decrease the coupling coefficient, and decrease the absolute value of TCF. SAW characteristics in the (100) AlN/64ºYX-$LiNbO_3$ structures with different electrical interfaces are investigated numerically. The effects of the polarity of the 64ºYX-$LiNbO_3$ substrate on SAW characteristics will be also discussed.

Keywords

(100) AlN; Temperature Coefficient of Frequency

Introduction

The use of thin films to improve the temperature stability, phase velocity, or coupling coefficient of a substrate has been proposed and implemented by many researchers. Hickernell has addressed the role that thin films play in surface acoustic wave (SAW) technology [1]. Yamanouchi and Ishii have deposited SiO_2 thin films on $LiNbO_3$ to produce a SAW device with high temperature stability and extremely high coupling [2]. Kadota has widely investigated the effects of ZnO thin films sputtered on different substrates such as glass and quartz [3]. Nakamura and Hanaoka have studied the propagation characteristics of SAWs in ZnO/128ºYX-$LiNbO_3$ structures [4]. SAW characteristics in AlN/128ºYX-$LiNbO_3$ structures have been measured by Wu *et al*. [5], [6] and numerically simulated by the authors [7]. The experimental results revealed that AlN films can increase the SAW velocity and decrease the absolute value of temperature coefficient of frequency (TCF), however, at the expense of a decrease in the coupling coefficient.

A 64ºYX◎ $LiNbO_3$ substrate has been used in the design of low loss, wide band, coupled resonator SAW filters owing to its large coupling coefficient (11.3%) and a high leaky SAW velocity (4742 m/s) but with a poor TCF (◎ 70 ppm/ºC) [8], [9]. AlN films have some excellent characteristics, including a high SAW velocity (5600 m/s), piezoelectricity, high temperature stability (TCF ≈ 30 ppm/ºC), and stable chemical stability [10], [11]. Recently, (100) AlN films have been deposited on different substrates including glass, Al_2O_3, and diamond [12]-[14]. Following the approach proposed by Campbell and Jones [15], [16] or the matrix method developed by Adler [17], phase velocity and coupling coefficient of SAWs in AlN/diamond structures have been evaluated [18], [19]. Results indicate that the maximum coupling coefficient is observed in the second mode, Sezawa mode. For example, in the (100) AlN/(111) diamond structure, the maximum coupling coefficient is 2.3% and the associated phase velocity is 10500 m/s, where the propagation direction is parallel to the *c*-axis and the *a*-axis is perpendicular to the diamond substrate [18]. These values are higher than those in the (002) AlN/(111) diamond, where the *c*-axis is perpendicular to the diamond substrate. Therefore, depositing (100) AlN films on 64ºYX-$LiNbO_3$ may provide a new piezoelectric material for SAW devices.

In this study, the reactive RF magnetron sputtering method is adopted for the growth of (100) oriented AlN films on 64ºYX-$LiNbO_3$. The crystalline structure of the AlN films is examined by the X-ray diffraction (XRD) method [20]. SAW devices with different films thickness-to-wavelength ratios are fabricated and characterized to investigate the SAW properties of this new composite substrate. The measured scattering parameters are employed to evaluate phase velocities and coupling coefficients of SAWs. The oscillation frequencies of SAW oscillators measured at different temperatures are used to calculate the TCF of SAWs. SAW characteristics in the proposed structures with different electrical interfaces are evaluated numerically. Simulation data show good agreement with measurement results. The effects of the polarity of the substrate on SAW characteristics will be also mentioned.

Experimental Procedure

AlN films are deposited by RF magnetron sputtering using a water-cooled 3-inch-diameter aluminum target (99.99%) in an argon/nitrogen gas mixture. The purity of the nitrogen gas is 99.995% and that of the argon gas is 99.99%. The sputtering parameters are presented in Table I. The crystalline structure and the crystallographic orientation of the AlN films are examined using a grazing incident angle XRD instrument (X'Pert PRO; PANalytical B.V., Almelo, The Netherlands). The power of XRD (CuK◎ radiation) is fixed at 45 kV and 40 mA. The incident angle of X-ray is fixed at 0.5º and the diffraction angle (2◎) ranges from 30º to 80º.

The SAW transversal filter, which consists of a pair of input and output interdigital transducers (IDTs), is fabricated on the top surface of the composite substrate ((100) AlN/64ºYX-$LiNbO_3$) by forming Al interdigital electrodes, which are deposited, patterned, and lifted via a conventional semiconductor process. Each transducer has 30 pairs of electrodes with uniform apodization. The overlap width is 5 mm. The width of electrode is 25◎ ◎ m and, hence, the wavelength, ◎ , is 100◎ m. The thickness of the Al electrode is 200 nm. The input and output IDTs are spaced 5 mm apart.

The SAW filters are characterized using a vector network analyzer (Model 8753E; Agilent Technology, Inc.). The averaged shifted velocity, v_a, is obtained from the equation $v_a = f_a \times$ ◎ , where f_a is the averaged shifted center frequency due to metallization [21]. The experimental electromagnetic coupling coefficient, K^2, is obtained using the following equation [22], [23].

$$K^2 = \frac{\pi}{4N}\frac{G_a}{B_a}\Big|_{f=f_a}, \qquad (1)$$

where N is the number of IDT finger pairs, and G_a and B_a are radiation conductance and susceptance, respectively, at f_a.

The oscillation frequencies of SAW oscillators, which consist of SAW transversal filters and amplifier circuits, at different temperatures are measured using a spectrum analyzer (Model E4403B; Agilent Technology, Inc.). The TCF is then evaluated via

$$TCF = \frac{f_r(35°C) - f_r(15°C)}{20°C \times f_r(25°C)}, \qquad (2)$$

where f_r(T°C) is the oscillation frequency at T°C.

TABLE 1 SPUTTERING PARAMETERS FOR DEPOSITING (100) ALN FILMS ON 64ºYX-$LiNbO_3$

Target-substrate distance (cm)	5 ~ 10
Base pressure (Torr)	10^{-6}
Sputtering pressure (m Torr)	3 ~ 9
RF power (W)	100 ~ 450
Substrate temperature (℃)	25 ~ 300
Nitrogen concentration (%) (N_2/ N_2+Ar)×100%	20 - 50
Total flow rate (sccm)	12

Theoretical Analysis

The layered piezoelectric structure, as schematically depicted in Fig. 1, comprises an (100) AlN layer of thickness h and a 64°Y $LiNbO_3$ substrate. Rayleigh or leaky SAWs are assumed to propagate along the x-axis. Following a similar approach to that developed by Campbell and Jones and others [15]-[17], a matrix method is employed to calculate the SAW velocity in the layered piezoelectric structure. Note that the matrix method may lead to numerical instabilities which may be resolved efficiently by the matrix algorithms described in [24], [25].

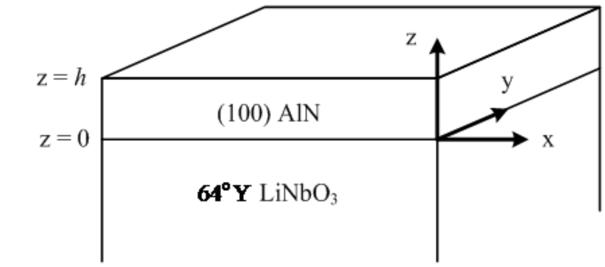


FIG. 1 SCHEMATIC OF A LAYERED PIEZOELETRIC STRUCTURE CONSISTING OF AN (100) ALN FILM OF THICKNESS *H* AND A 64ºY LINBO3 SUBSTRATE. RAYLEIGH OR LEAKY SAWS ARE ASSUMED TO PROPAGATE ALONG THE *X*-AXIS

The acoustic and electric fields in media 1 and 2 can be expressed as

$$u_j^{(1)} = \sum_{m=1}^{4} C_m a_j^{(m)} \exp\left(ikb^{(m)}z\right)\exp\left[ik\left(Px - vt\right)\right],\ j = 1,\ 2,\ 3, \tag{3}$$

$$\varphi^{(1)} = \sum_{m=1}^{4} C_m a_4^{(m)} \exp\left(ikb^{(m)}z\right)\exp\left[ik\left(Px - vt\right)\right], \tag{4}$$

$$u_j^{(2)} = \sum_{m=1}^{8} X_m \alpha_j^{(m)} \exp\left(ik\beta^{(m)}z\right)\exp\left[ik\left(Px - vt\right)\right], \tag{5}$$

$$\varphi^{(2)} = \sum_{m=1}^{8} X_m \alpha_4^{(m)} \exp\left(ik\beta^{(m)}z\right)\exp\left[ik\left(Px - vt\right)\right], \tag{6}$$

where u is the acoustic displacement, ϕ the electric potential, v the phase velocity, k the wave number in the x-direction, P = 1 + i◎, ◎ the attenuation coefficient, b and ◎ the wave number ratios, a and ◎ the corresponding eigenvectors, and C and ◎ the associated partial field amplitudes. Substituting (3) and (4) into stiffened Christoffel equations yields an eight-degree algebraic equation in the wave-number ratio b. Thus, for each pair of values of (v, ◎), there are eight real or complex values of b. For a semi-infinite piezoelectric crystal, medium 1 in this case, four complex roots with negative imaginary parts are selected for a Rayleigh wave; meanwhile, in the case of a leaky SAW, one complex root with a positive imaginary part is selected. In medium 2, all eight roots of are selected.

The boundary conditions require that the acoustic displacements and stresses be continuous at z = 0, and a stress-free surface is assumed at z = h. In addition, the electric potential and the normal component of electric displacement must be continuous at the interface for an electrically free surface. For a metalized (thin metal film) surface, the electric potential disappears. Substituting (3)-(6) into the boundary conditions, the phase velocity v and the attenuation coefficient ◎ can be obtained numerically.

The electromechanical coupling coefficient K^2 can then be calculated from

$$K^2 = 2\frac{v_f - v_m}{v_f}, \tag{7}$$

where v_f and v_m are phase velocities obtained when the electrical boundary conditions at the interface at which the IDT is placed are assumed to be electrically free and shorted, respectively.

The phase velocities and coupling coefficients are calculated for the following four cases according to the positions of the IDT electrodes and/or the thin metal films.

- IDT/AlN/64ºYX-LiNbO3,
- IDT/AlN/thin metal film/64ºYX-LiNbO3,
- AlN/IDT/64ºYX-LiNbO3, and
- Thin metal film/AlN/IDT/64ºYX-LiNbO3.

Results and Discussion

X-ray examination of piezoelectric films has been a major tool for determining the crystalline structure [20]. The XRD pattern of the AlN films on 64ºYX-LiNbO3 is shown in Fig. 2. The maximum peak at the diffraction angle of 33.218º confirms the (100) oriented crystalline structure of the AlN films according to the JCPDS (Joint of Committee on Power Diffraction Standards). Four SAW devices, named samples 1, 2, 3, and 4, are fabricated in this study; one of them, sample 1, is on the top surface of 64ºYX◎ LiNbO3 without AlN films and the rest three samples, denoted by samples 2, 3, and 4, are on the top surfaces of AlN/64ºYX-LiNbO3 with thicknesses of AlN films being equal to 0.5295, 1.1348, and 1.484m, respectively. The vector network analyzer and impedance analyzer are used to characterize these SAW devices. The middle frequency between first nulls in S21, which approximates the frequency at which the minimum S11 occurred, is adopted as the average shifted center frequency. The measured center frequencies of these four samples are 45.6625, 46.1305, 46.225, and 46.39375 MHz, respectively. The measured SAW velocities, $v_a = f_a \times$ ◎, plotted versus h/◎ are presented in Fig. 3 with open circle marks. It is clear that v_a increases as h/◎ increases.

Simulated SAW velocities in the IDT/AlN/64ºYX-LiNbO3 structure, named case (a) in this study, are also presented in Fig. 3. The material constants of AlN and LiNbO3 employed here are obtained from the studies

reported by Gualtieri *et al.* [10] and Kushibiki *et al.* [26]. Both v_f and v_m increase with increasing *h*/◎ in the entire *h*/◎ range of interest. This is because the Rayleigh wave velocity for (100) AlN, approximately 5646 m/s, is greater than the leaky SAW velocity for 64ºYX-$LiNbO_3$, 4742 m/s.

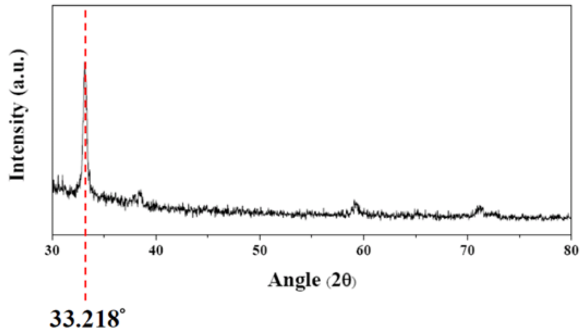


FIG. 2 THE XRD PATTERN OF THE ALN FILMS ON 64ºYX-LINBO3

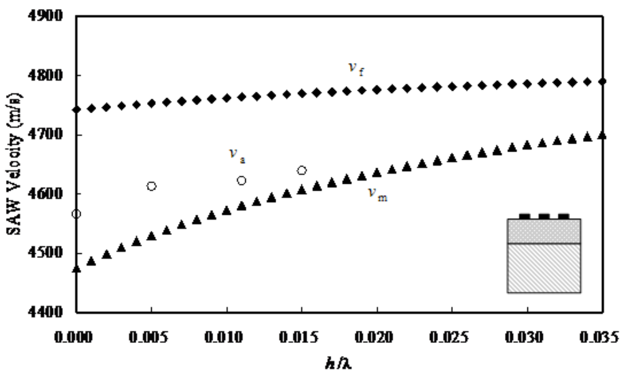
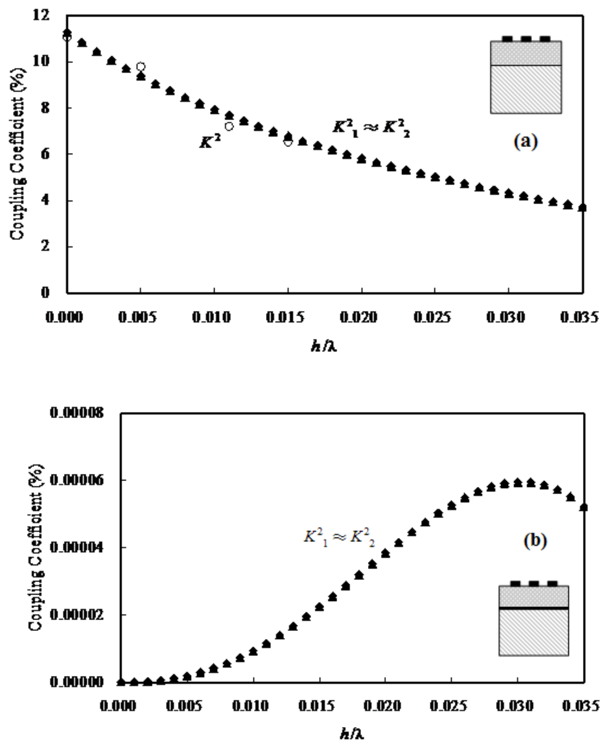


FIG. 3 MEASURED AND CALCULATED SAW VELOCITY VERSUS H/ FOR CASE (A) WITH AN IDT/(100) ALN/64ºYX-LINBO3 STRUCTURE. THE MEASUREMENT DATA ARE WITH OPEN CIRCLE MARKS

The experimental coupling coefficients evaluated by substituting measured impedances into (1) are presented in Fig. 4(a) open circle marks. The measured impedances at f_a obtained from the Smith chart of S11 for samples 1, 2, 3, and 4 are 31.649 + *i*7.487, 66.07 + *i*17.672, 121.67 + *i*44.164, and 74.609 + *i*29.879, respectively. The measured K^2 decreases from 11.07% for sample 1, 9.79% for sample 2, 7.21% for sample 3, to 6.54% sample 4 with increasing *h*/◎ .

With obtained v_f and v_m for cases (a) and (b), the coupling coefficients of SAWs for all four cases, cases (a)-(d), calculated using (7) are plotted in Figs. 4(a)-4(d). It is apparent that the simulated data presented in Fig. 4(a) are well matched with the measurement results. The subscripts 1 and 2 in K^2_1 and K^2_2 denote that the AlN films are deposited on the positive surface and the negative surface of the substrate, respectively. The angle between the positive surface normal and the *Y*-axis (crystallographic coordinate) is 64º, while for the negative surface it is ◎ 116º as schematically depicted in Fig. 5. For all the cases shown in Figs. 4(a)-4(d), $K^2_1 \approx K^2_2$, which illustrates that in the (100) AlN/64ºYX-$LiNbO_3$ structures the effects of the polarity of the 64ºYX-$LiNbO_3$ substrate can be ignored. This result is significantly different from that found in the (002) ZnO/128ºYX-$LiNbO_3$ structures [4] or in the (002) AlN/128ºYX-$LiNbO_3$ structures [7].

In Fig. 4(a) or 4(c), the coupling coefficient decreases monotonically with increasing *h*/◎ . The decreasing rate of the coupling coefficient in Fig. 4(a), case (a), is much greater than that in the case of (c), Fig. 4(c). In Fig. 4(b), the coupling coefficient has a very small value compared with the rest three cases. This illustrates that the thin metal film deposited on the interface plane between the two piezoelectric media decreases the coupling coefficient significantly. The coupling coefficient in the case of (d) is presented in Fig. 4(d). In the entire *h*/◎ range, K^2 increases monotonically and its value is smaller than that in Fig. 4(c). This shows that a thin metal film deposited on the upper surface may also decrease the coupling coefficient. According to the simulation data presented in Figs. 4(a)-4(d), the AlN/IDT/64ºYX-$LiNbO_3$ structure exhibits the largest coupling coefficient of all the cases investigated in this study.



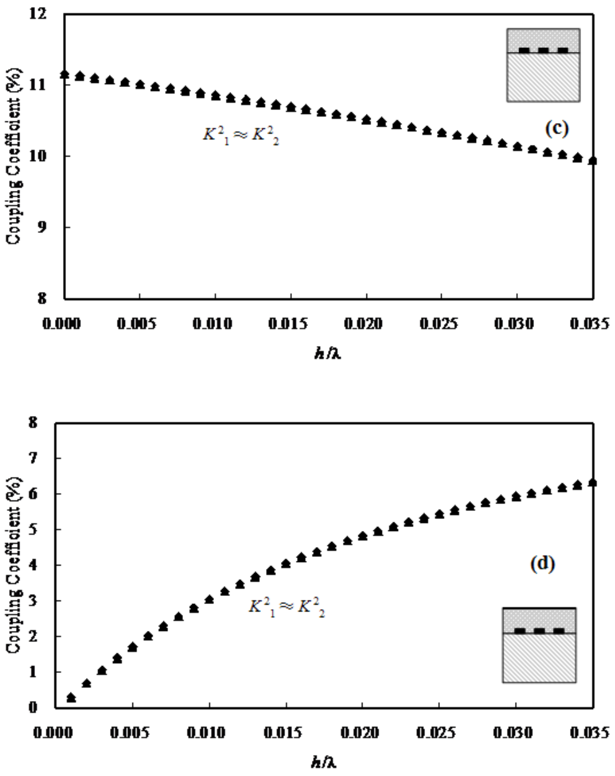


FIG. 4 MEASURED AND CALCULATED SAW COUPLING COEFFICIENTS: (A) CASE (A), CALCULATED DATA ARE WELL MATCHED WITH EXPERIMENTAL RESULTS. (B) CASE (B), THE COUPLING COEFFICIENT IN THIS CASE IS THE SMALLEST OF THE FOUR CASES STUDIED, (C) CASE (C), THE COUPLING COEFFICIENT IN THIS CASE IS THE LARGEST OF THE FOUR CASES STUDIED, AND (D) CASE (D)

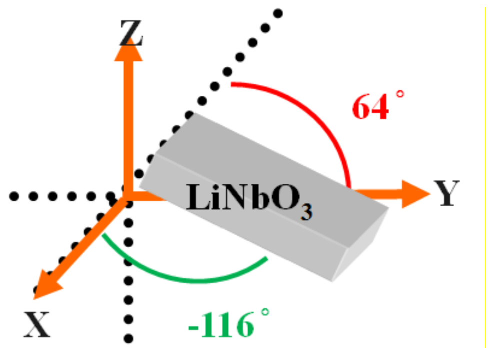


FIG. 5 THE ANGLE BETWEEN THE POSITIVE SURFACE NORMAL AND THE *Y*-AXIS (CRYSTALLOGRAPHIC COORDINATE) IS 64º, WHILE FOR THE NEGATIVE SURFACE IT IS 116º

The measured oscillation frequencies of all four SAW oscillators at 15, 25, and 35ºC obtained using a spectrum analyzer are substituted into (2) to evaluate the experimental TCF. The corresponding data are presented in Table II. It is apparent that the absolute of TCF decreases with increasing $h/⊚$. This is because AlN has a positive TCF and the 64ºYX-$LiNbO_3$ substrate has a negative TCF.

TABLE 2 MEASURED OSCILLATION FREQUENCY AND TCF

Sample	Oscillation frequency (MHz)			TCF (ppm/ºC)
	15ºC	25ºC	35ºC	
1	45.6392	45.6107	45.5822	⊚ 62.49
2	46.2584	46.2317	46.2042	⊚ 58.62
3	46.3626	46.3379	46.3131	⊚ 53.41
4	46.4158	46.3956	46.3693	⊚ 50.11

Conclusions

In this study, (100) AlN films are deposited on the 64ºYX-$LiNbO_3$ substrate by the RF magnetron sputtering method to form a new piezoelectric substrate. SAW devices fabricated on the new composite substrate with different AlN films thicknesses are characterized. Phase velocity and coupling coefficient of SAWs in the (100) AlN/64ºYX-$LiNbO_3$ structures are simulated and compared with measurement data. The simulation results show good agreement with the measurement data. The research results illustrate that the increase of the thickness of AlN films will increase the SAW velocity, decrease the coupling coefficient, and decrease the absolute value of TCF. According to the simulation data, the AlN/IDT/64ºYX-$LiNbO_3$ structure exhibits the largest coupling coefficient of all the cases investigated in this study. It is also shown that in the (100) AlN/64ºYX-$LiNbO_3$ structures the effects of the polarity of the 64ºYX-$LiNbO_3$ substrate can be ignored.

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